Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

**Rational Band Structure Engineering of $TiO_2$ for Photoelectrochemical Water Splitting** SU-HUAI WEI, WAN-JIAN YIN, YANFA YAN, National Renewable Energy Lab — The search for new semiconducting materials or the engineering of existing semiconductors for commercially viable photoelectrochemical (PEC) water splitting has been extremely challenging. Meeting that challenge requires the discovery of a semiconductor with several tightly coupled material property criteria such as appropriate band gap (1.6 – 2.2 eV), efficient visible light absorption, high carrier mobility, and correct band edge positions that straddle the water redox potentials. However, previous searches/modifications of semiconducting materials for PEC water splitting application have often focused on a particular individual criterion such as band gap, neglecting the possible detrimental consequence to other important criteria. In this talk, general strategies for the rational design of semiconductors such as $TiO_2$ to simultaneously meet all of the requirements for a high efficiency solar-driven PEC water splitting device are discussed. Density-functional theory calculations reveal that with appropriate donor-acceptor co-incorporation, heavily doped anatase $TiO_2$ hold great potential to satisfy all of the criteria for a viable PEC device. Other approaches to modify the band structure of $TiO_2$, such as the application of strain, will also be discussed.

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Date submitted: 24 Nov 2010 Electronic form version 1.4